Momentum distribution of an interacting Bose-condensed gas at finite temperature

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We use a semiclassical two-fluid model to study the momentum distribution of a Bose-condensed gas with repulsive interactions inside a harmonic trap at finite temperature, with specific focus on atomic hydrogen. We give particular attention to the average kinetic energy, which is almost entirely associated with the thermal cloud. A non-linear dependence of the kinetic energy on temperature is displayed, affording a precise way to assess the temperature of the gas. We also show that the kinetic energy increases with the strength of the interactions, reflecting an enhanced rate of depletion of the condensate with increasing temperature.

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I. INTRODUCTION

The observation in momentum space of Bose-Einstein condensation in a trapped gas with repulsive interactions presents at least in principle some advantage over observation in coordinate space. Since the condensate belongs to a single quantum state, a broadening of its density profile implies a narrowing of its momentum distribution. At the same time the width of the momentum distribution of the thermal cloud is in essence unchanged, the role of quantal indeterminacy being negligible for this component.

The momentum distribution of a dilute Bose-condensed gas has been measured both on trapped and expanding vapours of ^{23}Na at $T \simeq 0$ [1] and on trapped vapours of spin-polarized ^{1}H atoms at finite temperature [2]. The former experiment has been successfully interpreted by means of a Thomas-Fermi model [3,4]. In the present work we are concerned with the latter experiment, in which the momentum distribution of the hydrogen cloud was inferred from the Doppler-sensitive part of the $1S$-$2S$ two-photon absorption spectrum: the measured distribution shows a small condensate peak on top of a broad thermal component. Cold collisions in the high-density condensate broaden the peak associated with it [5,6]. Here we are instead interested in extracting thermodynamic information on the system from the thermal part of the spectrum.

We use a semiclassical two-fluid model, which was earlier developed to account for the release energy in expanding clouds of ^{87}Rb as a function of temperature [7]. With this model we evaluate the momentum distribution of an interacting Bose gas at equilibrium under harmonic confinement. The results for a choice of parameters corresponding to the experiment on hydrogen agree with the measured condensate fraction within its error bars. We place particular attention on the average kinetic energy of the gas, displaying its temperature dependence and the role of the interactions.

Before proceeding we should mention that, in addition to the Doppler-sensitive part of present interest, the measured spectrum also includes a Doppler-free contribution. The thermal portion of this Doppler-free spectrum has been interpreted within an out-of-equilibrium picture invoking large fluctuations in the particle density [8]. However, the contribution of such fluctuations to the Doppler-sensitive thermal spectrum is expected to be of the same order as for the Doppler-free line, making it smaller than the Doppler broadening by two orders of magnitude.

II. THE MODEL AND ITS JUSTIFICATION

In our description of the Bose gas with repulsive interactions, confined in a harmonic trap at finite temperature T, we adopt the semiclassical Hartree-Fock (HF) scheme for the thermal cloud and the Thomas-Fermi (TF) approximation for the condensate.

The choice of a mean field theory is justified by the fact that in current experiments the gas is in a very dilute regime, corresponding in the trap to the condition $N^{1/6}a/a_{ho} \ll 1$ [9] where N is the number of particles, a is the s-wave scattering length and $a_{ho} = (\hbar/m\omega)^{1/2}$ is the harmonic oscillator length. Here $\omega = (\omega_\perp^2\omega_z)^{1/3}$ is the geometrical average of the harmonic oscillator frequencies characterizing the axially symmetric confining potential $V_{ext}(\mathbf{r}) = m(\omega_\perp^2 r_\perp^2 + \omega_z^2 z^2)/2$. In particular, in the hydrogen experiment $N^{1/6}a/a_{ho} \simeq 0.001$.

In the presence of confinement the HF scheme has been shown to provide a simple and accurate description of the excitation spectrum [10], yielding results which are comparable with the predictions of the full Bogoliubov theory.

The semiclassical approximation is valid for a bosonic cloud when its temperature is appreciably larger than the harmonic-oscillator spacing, $k_BT \gg \hbar\omega_{\perp,z}$. In particular, in the hydrogen experiment $k_BT \simeq 270\hbar\omega_\perp \simeq 10^5\hbar\omega_z$. For the specific case of trapped atomic vapours, the semiclassical HF approximation has also been tested by a Monte Carlo calculation [11], performed with a choice of parameters corresponding to the ^{87}Rb experiments [12].

The TF approximation for the condensate well describes the gas with repulsive interactions in the strong coupling limit $N_c\, a/a_{ho} \gg 1$, *i.e.* when the number N_c of atoms in the condensate is large. This approximation is therefore valid everywhere except in the critical region. In the hydrogen experiment one has $N_c a/a_{ho} \simeq 1.6 \cdot 10^4$.

On all these counts, therefore, the use of the semiclassical two fluid model is fully justified in the calculations that we present below, except in the immediate neighbourhood of the critical temperature as remarked just above. The momentum distributions of the thermal cloud $f_T(\mathbf{p})$ and of the condensate $f_c(\mathbf{p})$ are then given by the Bose distribution in an effective potential and by the square modulus of the Fourier transform of the wavefunction of the condensate:

$$f_T(\mathbf{p}) = \int \left\{ \exp\left[\frac{1}{k_BT}\left(\frac{p^2}{2m} + V_{eff}(\mathbf{r}) - \mu\right)\right] - 1 \right\}^{-1} \mathrm{d}^3\mathbf{r} \ , \tag{1}$$

and

$$f_c(\mathbf{p}) = \left| \int \phi_c(\mathbf{r}) e^{-i\mathbf{p}\cdot\mathbf{r}} \mathrm{d}^3\mathbf{r} \right|^2 \ . \tag{2}$$

Here $\phi_c(\mathbf{r}) = \sqrt{n_c(\mathbf{r})}$, the square root of the density profile of the condensate. In Eq. (1) the effective potential acting on the thermal cloud is given by

$$V_{eff}(\mathbf{r}) = V_{ext}(\mathbf{r}) + 2gn_c(\mathbf{r}) + 2gn_T(\mathbf{r}) \ , \tag{3}$$

$n_T(\mathbf{r})$ being the density profile of the thermal cloud. Finally, we have

$$n_c(\mathbf{r}) = \frac{1}{g} \left[\mu - V_{ext}(\mathbf{r}) - 2gn_T(\mathbf{r})\right] \theta(\mu - V_{ext}(\mathbf{r}) - 2gn_T(\mathbf{r})) \tag{4}$$

and

$$n_T(\mathbf{r}) = \int \left\{ \exp\left[\frac{1}{k_BT}\left(\frac{p^2}{2m} + V_{eff}(\mathbf{r}) - \mu\right)\right] - 1 \right\}^{-1} \frac{\mathrm{d}^3\mathbf{p}}{(2\pi)^3}. \tag{5}$$

The coupling constant g is fixed by the s-wave scattering length a through the relation $g = 4\pi\hbar^2 a/m$, and the chemical potential μ is fixed by the total number N of atoms,

$$\int \left[n_c(\mathbf{r}) + n_T(\mathbf{r})\right] \mathrm{d}^3\mathbf{r} = N \ . \tag{6}$$

For temperatures above the critical condensation temperature the expression (1) is equivalent to that developed by Chou *et al.* [14].

III. MOMENTUM DISTRIBUTIONS

In the experiments of Fried et al. [2] on atomic hydrogen the momentum distribution has been inferred from the Doppler-sensitive spectrum as measured along the weakly confining axis of the trap. We accordingly report in Figures 1 and 2 the distributions for the thermal cloud and for the condensate as functions of the axial momentum p_z:

$$F_{T,c}(p_z) = \int \frac{\mathrm{d}^2 p_\perp}{(2\pi)^2} f_{T,c}(\mathbf{p}). \tag{7}$$

The units of length and momentum are $a_{ho\perp} = (\hbar/m\omega_\perp)^{1/2}$ and $p_{ho\perp} = (\hbar m\omega_\perp)^{1/2}$, with the values of m and $\omega_\perp$ of the experiment [2]. We have taken $\omega_\perp = 2\pi \cdot 3.9$ kHz and $\omega_z = 2\pi \cdot 10.2$ Hz.

Figure 1 illustrates both the role of statistics and the effect of the interactions on the axial momentum distribution of the thermal component. The predictions of the semiclassical model for a weakly interacting gas, with a scattering length chosen equal to that of ^{1}H ($a_H = 6.48 \cdot 10^{-2}$ nm from accurate calculations by Jamieson *et al.* [13]) or arbitrarily

increased to $20\,a_H$ for illustrative purposes, are compared with each other and with that for a non-interacting Bose gas. The value of the temperature is $T = 50.3\,\mu$K, as will be discussed in Sect. IV below. Figure 1 also reports the momentum distribution of the classical gas at the same temperature.

It is evident from Figure 1 that quantum statistics increases the population of the states at low momentum, as expected. The main effect of the interactions is instead a depletion of the condensate, leading to increases in the population and in the width of the momentum distribution of the thermal cloud.

The momentum distribution of the condensate at the same temperature as coming from the Thomas-Fermi model is shown in Fig. 2.

IV. KINETIC ENERGY

We proceed to study the momentum distribution of an interacting Bose gas as a function of temperature by focusing on its second moment, that is on the kinetic energy of the trapped cloud. This is the quantity which can be most directly compared with the experimental data [2].

In Figure 3 we show the behaviour of the kinetic energy of the gas for two values of the scattering length, corresponding to the experimental value $a = a_H$ for the hydrogen gas and to the stronger interaction $a = 20a_H$, as compared with the non-interacting quantum and classical results. For the parameters corresponding to the hydrogen experiment the effect of the interactions on the kinetic energy is clearly quite negligible. Indeed, the dilution parameter for this system is very small, $N^{1/6}a_H/a_{ho} \simeq 0.001$ as already noted. On increasing the interaction strength we find that the kinetic energy increases. This effect can be understood as coming from enhanced depletion of the condensate. There is instead a major effect of quantal statistics on the average kinetic energy below the condensation temperature, as is seen from Figure 3.

It is important to stress that in the interacting gas the behaviour of the kinetic energy depends not only on the scattering length but also on the total number of particles in the system. This is illustrated in Figure 4. We have exploited this fact to test how far the semiclassical model can quantitatively explain the experimental results of Fried *et al.* [2] on the hydrogen gas. After choosing a value for the total number of particles in the cloud within the experimental error bars, we have fitted to experiment the calculated kinetic energy and extracted from the model the temperature of the cloud and the condensate fraction. For a total number of atoms equal to $N = 10.5 \cdot 10^9$ we obtain $N_c/N = 10\%$, that is $N_c = 1.05 \cdot 10^9$ at a temperature $T = 50.3\ \mu$K. The experimental values are $N_c/N = 6^{+6}_{-3}\%$ and $N_c = 1.1 \pm 0.6 \cdot 10^9$. Therefore, we conclude that the semiclassical model is compatible with the experimental data for the momentum distribution of the thermal cloud.

Our calculations also show that from kinetic energy data it is possible, through the semiclassical model to obtain a good estimate for the temperature of the Bose cloud below the critical temperature. In the intermediate- to low-temperature region this procedure yields a result which differs significantly from the classical result $E^z_{kin} = k_BT/2$. For the specific case of the hydrogen experiment we estimate that the value of the temperature corresponding to the measured kinetic energy is $T = 50.3\,\mu$K, that is about 20% higher than the value extrapolated from the classical result (see again Figure 3).

V. SUMMARY AND CONCLUSIONS

In summary, the Doppler-sensitive part of the $1S$-$2S$ two-photon absorption spectrum of Bose-condensed atomic hydrogen contains quantitative information on thermodynamic properties, which can be extracted from the available data by means of an analysis combining a Thomas-Fermi treatment of the condensate with a semiclassical Hartree-Fock treatment of the thermal cloud. The spectral broadening due to fluctuations in the density is negligible and the spectral width is directly related to the kinetic energy of the gas.

Within such a semiclassical two-fluid model we have studied the momentum distribution and the mean kinetic energy of a Bose-condensed gas with repulsive interactions. From the behaviour of the kinetic energy as a function of temperature and of the coupling strength we have reached two main conclusions: (i) the interactions enhance the rate of depletion of the condensate with increasing temperature, causing an increase of the kinetic energy; and (ii) the relation between kinetic energy and temperature is strongly non-linear, owing to the role of quantal statistics as opposed to classical statistics. It appears that the present model may yield useful improvements in the analysis of experimental data.

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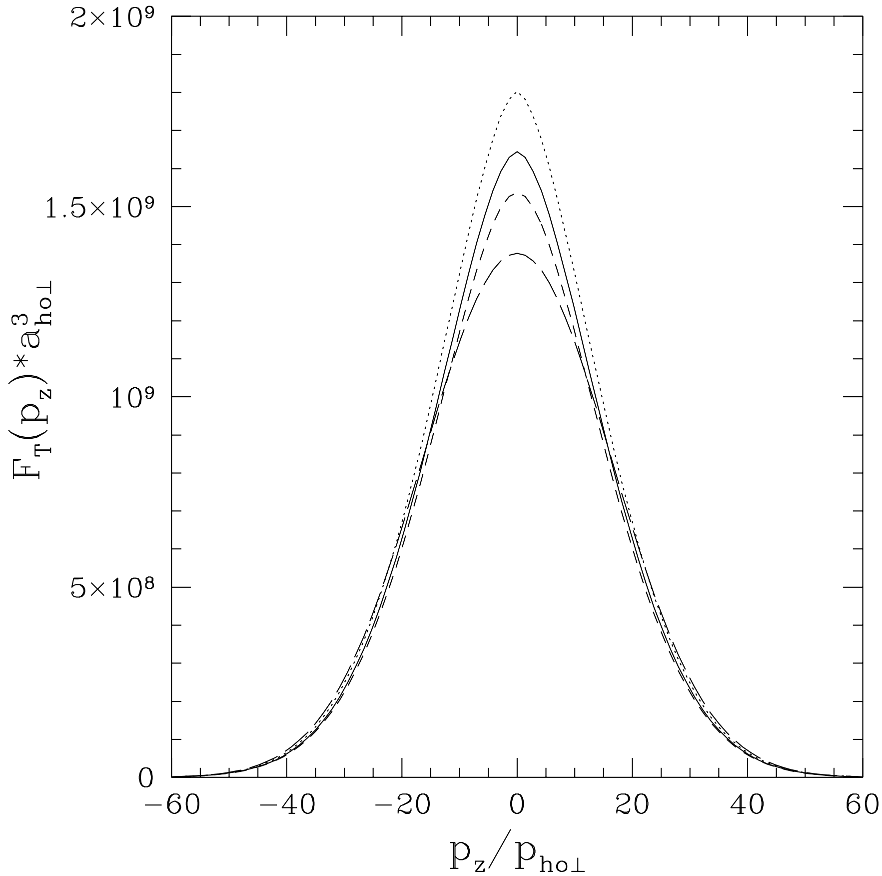

FIG. 1. Axial momentum distribution of the thermal component of a weakly interacting Bose gas with $N = 10.5 \cdot 10^9$ at $T = 50.3\,\mu$K. The scattering length is $a = 20a_H$ (dotted curve) and $a = a_H$ (continuous curve) with $a_H = 6.48 \cdot 10^{-2}$ nm. These two curves are compared with the momentum distribution of the non-interacting Bose gas (dashed curve) and of the classical gas (long-dashed curve). The latter has the same number of particles as the non-interacting quantal gas.

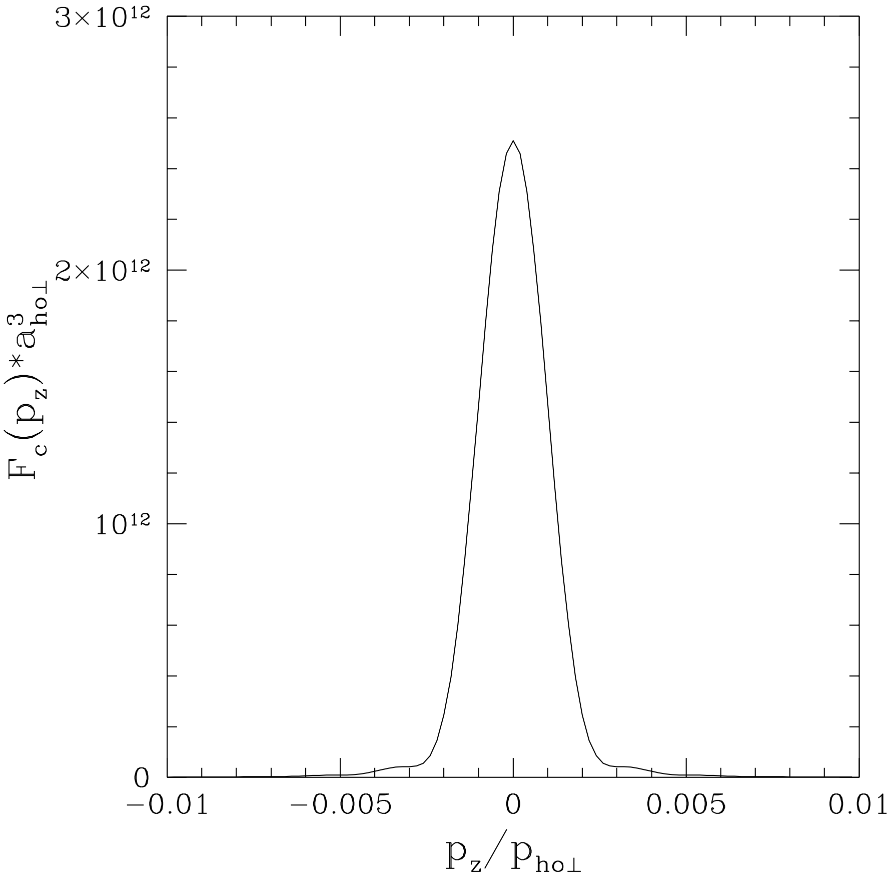

FIG. 2. Axial momentum distribution of the condensate in an interacting Bose gas with $N = 10.5 \cdot 10^9$ at $T = 50.3\mu$K. The scattering length is $a = a_H$.

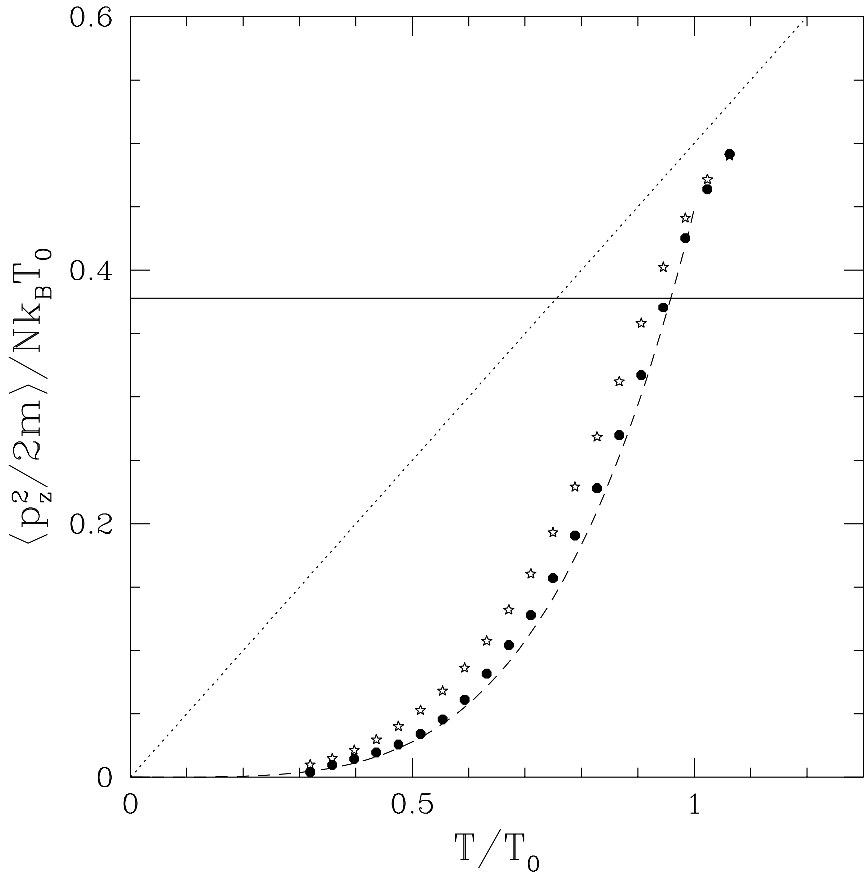

FIG. 3. Kinetic energy versus temperature (in units of the ideal-gas critical temperature T_0) for an interacting Bose gas with $N = 10.5 \cdot 10^9$ at a scattering length $a = 20a_H$ (stars) and at the hydrogen scattering length (filled circles). These results are compared with the kinetic energy of the non-interacting Bose gas (dashed curve) and of the classical gas (dotted curve). The horizontal full line locates the kinetic energy measured in the hydrogen experiment [2].

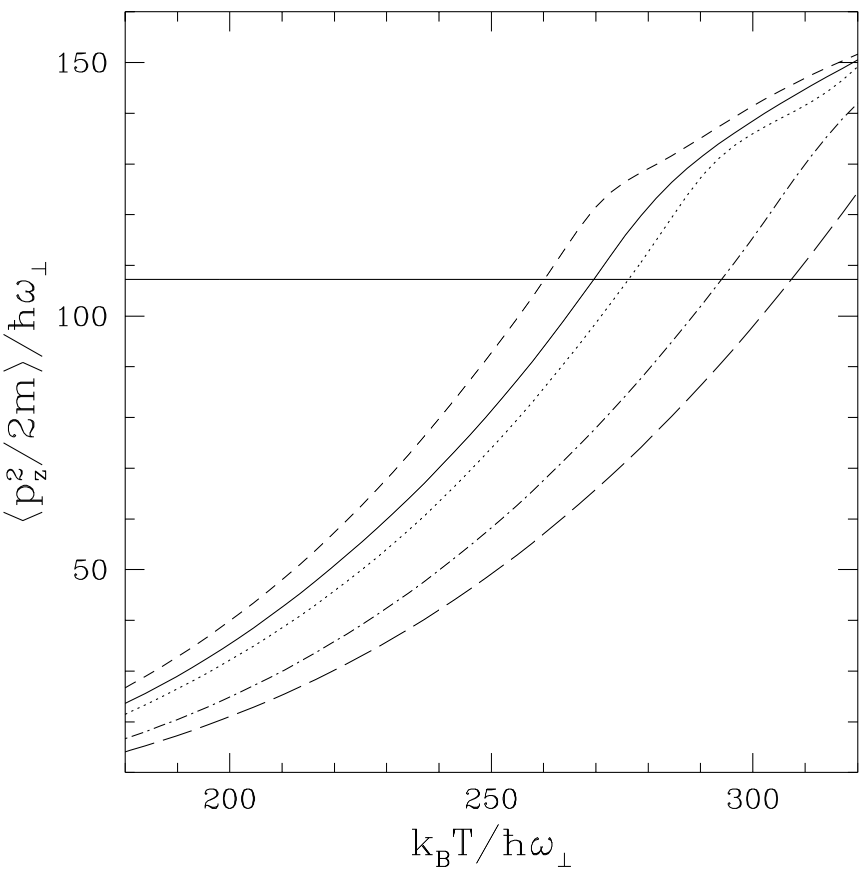

FIG. 4. Kinetic energy versus temperature for an interacting Bose gas at different values of the total number of particles: $N = 18.3 \cdot 10^9$ (long-dashed), $N = 15 \cdot 10^9$ (dashed-dotted), $N = 11.6 \cdot 10^9$ (dotted), $N = 10.5 \cdot 10^9$ (continuous) and $N = 9.5 \cdot 10^9$ (short-dashed). The horizontal full line locates the kinetic energy measured in the hydrogen experiment [2].